16. CLASS OF G_{16} - ESTIMATORS IN THE THEORY OF EXPERIMENTAL DESIGN, WHEN THE DESIGN MATRIX IS UNKNOWN

In this section we deal with problems of experimental design under the G-condition

$$\limsup_{n\to\infty} m_n n^{-1} < \infty.$$

Such a condition occurs when the number m of unknown parameters is large, and the number of experiments n has the same order. Given the G-condition, the evaluation of every separate parameter a_i yields under some standard conditions the value $c_1 n^{-1/2}$, where c_1 is some constant. In some cases, the total evaluation error is $c_1 m n^{-1/2}$.

In view of the above, it seems that it is impossible to obtain consistent estimators under the G-condition. However, for many problems it is necessary to evaluate not the parameters a_i, but some function of these parameters $f(a_1,\ldots,a_m)$. But it turns out that in many cases it is possible to find the limit of this function as $n\to\infty$;

$$\limsup_{n\to\infty} \left| f(\hat{a}_1,\ldots,\hat{a}_m) - g(a_1,\ldots,a_m)\right| = 0.$$

The function g is known and can be obtained as the solution of some equation. This function g differs from the true function f, but when these two functions are known, we can find the G-estimator $G(\hat{a}_1,\ldots,\hat{a}_m)$ of function $f(a_1,\ldots,a_m)$ such that in probability or with probability one, the following limit is valid

$$\limsup_{n\to\infty} \left| G(\hat{a}_1,\ldots,\hat{a}_m) - f(a_1,\ldots,a_m)\right| = 0.$$

A brief outline of applications of the G-analysis methods described in this section follows.

16.1. G_{16} -estimator of regression models errors. The resolvent method in the theory of experiment design, when the design matrix is random

Let us consider the regression model

$$\vec{y} = X\vec{c} + \vec{\varepsilon},\ \mathbf{E}\,\vec{\varepsilon} = \vec{0},\ \ \mathbf{E}\,\vec{\varepsilon}\vec{\varepsilon}^T = R_{m_n},\ \ \mathbf{E}\,X = A$$

where X is a random matrix, A is a known matrix and the distribution of the matrix X is unknown. Only a simple characteristic of this distribution is known, namely: the entries of the matrix X are independent and their variances are equal to certain constants. Consider a regularized estimator of parameters of this linear regression model

$$\vec{c}_\alpha = \left(\alpha I + X^T X\right)^{-1} X^T \vec{y}. \tag{16.1}$$

Suppose that we have performed experimental design under the random matrix X, which does not depend on the random vector $\vec{\varepsilon}$. Then

$$\vec{c} - \vec{c}_\alpha = \vec{c} - \left\{\alpha I + X^T X\right\}^{-1} X^T \vec{y}.$$

Let $\alpha = 0,\ \mathbf{E}\,\vec{\varepsilon}_i = 0,\ \mathbf{Cov}\,\varepsilon_i\varepsilon_i = n^{-1}\delta_{ij}$ and $p\liminf\limits_{n\to\infty} \lambda_{\min}\left\{X^T X\right\} > 0$. We have

$$\mathbf{E}\left\{\|\vec{c} - \vec{c}_\alpha\|_{\alpha=0} | X\right\} = n^{-1}\mathrm{Tr}\left\{X^T X\right\}^{-1}.$$

Such an expression is inconvenient for finding a minimum on some set of matrices X, since X is a random matrix. It can happen that this matrix will be ill-posed with a positive probability. Therefore it is very important that under general conditions this expression converges to some nonrandom expression, which is more convenient for finding the optimum design. We introduce here the G_{16} estimator of this error $\mathbf{E}\left\{\|\vec{c}-\vec{c}_\alpha\|_{\alpha=0}\,|X\right\}$:

$$G_{16} = b_n\left(0\right),$$

where real analytic function $b_n\left(\alpha\right), \alpha > 0$ satisfies the following equation

$$b_n\left(\alpha\right) = \frac{1}{n}\mathrm{Tr}\left\{I\left[1+\gamma b_n\left(\alpha\right)\right] + (1-\gamma) + \frac{1}{1+\gamma b_n\left(\alpha\right)}AA^T\right\}^{-1}, \gamma = \frac{m_n}{n} < 1.$$

We mean here the G_{16}–estimator of the expression for $\mathbf{E}\left\{\|\vec{c}-\vec{c}_0\|\,|X\right\}$.

THEOREM 16.1. *If for every n the random entries x_{ij} of the matrix X are independent,*

$$\mathbf{E}\,x_{ij} = a_{ij}, \quad \mathbf{Var}\,x_{ij} = n^{-1}, \quad \limsup_{n\to\infty} m_n^{-1}n < 1, \quad \mathbf{E}\left|(x_{ij}-a_{ij})\sqrt{n}\right|^{4+\delta} \le c < \infty, \ \delta > 0,$$

$$0 < c_1 \le \lambda_k(AA^T) \le c_2 < \infty,$$

then

$$p\lim_{n\to\infty}\left[\mathbf{E}\left\{\|\vec{c}-\vec{c}_\alpha\|_{\alpha=0}\,|X\right\} - G_{16}\right] = 0.$$

16.2. G_{16} -estimator of regression models errors. The resolvent method in the theory of experiment design, when the design matrix is an observation of a certain random matrix

Let us consider the regression model

$$\vec{y} = A\vec{c} + \vec{\varepsilon}, \ \mathbf{E}\,\vec{\varepsilon} = \vec{0}, \quad \mathbf{E}\,\vec{\varepsilon}\vec{\varepsilon}^T = R_{m_n},$$

where A is a matrix.

Here, under the same conditions as in the previous section, we consider the following quality criterion of the least squares estimator

$$\mathbf{E}\left\{\|\vec{c}-\vec{c}_\alpha\|_{\alpha=0}\right\} = n^{-1}\mathrm{Tr}\left\{A^TA\right\}^{-1}.$$

Suppose that we do not know the matrix A, but we have one observation of the matrix X, where X is a random matrix not depending on random vector $\vec{\varepsilon}$ such that $\mathbf{E}\,X = A$. Then the G_{16} estimator of this error, $n^{-1}\mathrm{Tr}(A^TA)^{-1}$, is equal to:

$$G_{16}(B,C,u+\mathrm{i}v) = \mathrm{i}\int_0^B \left\{\frac{\mathrm{e}^{|sp|}}{\pi}\int_{-C}^{C}\mathrm{Im}\,G_{27}(z)\mathrm{e}^{-\mathrm{i}tp}\mathrm{d}t\right\}\mathrm{e}^{-p(v-\mathrm{i}u0}\mathrm{d}p, \quad v > 0.$$

Here the G_{27}-estimator of Stieltjes' transform (see Section 27)

$$\varphi\left(z, AA^T\right) = m^{-1}\mathrm{Tr}\left[AA^T - zI_{m_n}\right]^{-1}$$

is by definition the following expression:

$$G_{27}\left(\alpha, XX^T\right) = \varphi\left(\hat{\theta}(z), XX^T\right)\left[1+\gamma\varphi\left(\hat{\theta}(z), XX^T\right)\right]^{-1},$$

where $\hat{\theta}(z)$ is the measurable solution of the G_{27} equation

$$\begin{aligned} &-\hat{\theta}(z)\left\{1+\frac{1}{n}\mathrm{Tr}\left[XX^T-\hat{\theta}(z)I_{m_n}\right]^{-1}\right\}^2 \\ &+\left(1-\frac{m_n}{n}\right)\left\{1+\frac{1}{n}\mathrm{Tr}\left[XX^T-\hat{\theta}(z)I_{m_n}\right]^{-1}\right\} = -z, \end{aligned}$$

$z = t + \mathrm{i}s,\ s > c$ and c is a certain constant.

THEOREM 16.2. *If the conditions of Theorem 16.1 are fulfilled, then*

$$\lim_{\nu\downarrow 0}\lim_{B\to\infty}\lim_{C\to\infty} p\lim_{n\to\infty}\left|n^{-1}\mathrm{Tr}(A^TA)^{-1} - G_{16}(B, C, 0+\mathrm{i}\nu)\right| = 0.$$

16.3. The G_{16} -estimator of regularized regression models errors. The resolvent method in the theory of experiment design, when the design matrix is random

Let us consider the regression model

$$\vec{y} = X\vec{c} + \vec{\varepsilon},\ \mathbf{E}\,\vec{\varepsilon} = \vec{0},\ \mathbf{E}\,\vec{\varepsilon}\vec{\varepsilon}^T = R_{m_n},\ \mathbf{E}\,X = A$$

where X is a random matrix, A is a known matrix and the distribution of the matrix X is unknown. Only simple characteristics of this distribution are known, namely: the entries of the matrix X are independent and their variances are equal to certain constants. Consider a regularized estimator of parameters of this linear regression model

$$\vec{c}_\alpha = \left(\alpha I + X^TX\right)^{-1} X^T\vec{y}. \tag{16.2}$$

Suppose that we have performed experimental design under the random matrix X, which does not depend on random vector $\vec{\varepsilon}$. Then

$$\begin{aligned} \vec{c} - \vec{c}_\alpha &= \vec{c} - \left\{\alpha I + X^TX\right\}^{-1} X^T\vec{y} \\ &= \vec{c} - \left\{\alpha I + X^TX\right\}^{-1} X^TX\vec{c} - \left\{\alpha I + X^TX\right\}^{-1} X^T\vec{\varepsilon} \\ &= \alpha\left\{\alpha I + X^TX\right\}^{-1}\vec{c} - \left\{\alpha I + X^TX\right\}^{-1} X^T\vec{\varepsilon}. \end{aligned}$$

Suppose that the unknown vector $\vec{c}$ satisfies the inequality $\vec{c}^TD\vec{c} \le 1$, where D is a positive defined symmetric matrix. Then we can use the spectral theory of estimation of unknown parameters [Gir84] to find the following regression model error:

$$\begin{aligned} \max_{\vec{c}^TD\vec{c}\le 1}\mathbf{E}\,(\vec{c}-\vec{c}_\alpha)(\vec{c}-\vec{c}_\alpha) &= \alpha\lambda_{\max}\left\{D^{-1/2}\left\{\alpha I + X^TX\right\}^{-2} D^{-1/2}\right\} \\ &\quad + \mathrm{Tr}\left\{\alpha I + X^TX\right\}^{-2} X^TRX. \end{aligned}$$

For simplification we have assumed $D = I$. Now we transform this expression to such a form for which it will be easy to apply the methods of GSA:

$$\max_{\vec{c}^T D\vec{c}\le 1} \mathbf{E}\left(\vec{c}-\vec{c}_\alpha\right)\left(\vec{c}-\vec{c}_\alpha\right)=\alpha\left\{\alpha+\lambda_{\min}\left[X^T X\right]\right\}^{-2}$$
$$-\frac{\partial}{\partial\gamma} n^{-1}\mathrm{Tr}\left\{\alpha I+X^T\left(I+\gamma R\right)X\right\}^{-1}_{\gamma=0}.$$

For further simplification we will assume that $R=In^{-1}$ and matrix x satisfies the conditions of Theorem 16.1. Then the G_{16} estimator of regression model error is introduced as follows:

$$G_{16}=\alpha\left[\alpha+\beta_1\right]^{-2}+\alpha\frac{\partial b_n(\alpha)}{\partial\alpha}+b_n(\alpha),$$

where

$$\beta_1=\max\left\{0,\ (1-\gamma)\left[1-\frac{\gamma}{m}\sum_{k=1}^{m}\frac{1}{\alpha_k-v_s}\right]+v_s\left[1-\frac{\gamma}{m}\sum_{k=1}^{m}\frac{1}{\alpha_k-v_s}\right]^2\right\},$$

and v_s are certain real solutions of the L_2 equation (see Chapter 4)

$$1-\sum_{k=1}^{m}\frac{\gamma}{m\left(\alpha_k-v_i\right)}=\left[\sum_{k=1}^{m}\frac{\gamma}{m\left(\alpha_k-v_i\right)^2}\right]\left\{\frac{1-\gamma}{1-\sum\limits_{k=1}^{m}\frac{\gamma}{m(\alpha_k-v_i)}}+2v_i\right\},$$

α_k are the eigenvalues of the matrix AA^T and $b_n(\alpha)$ satisfies the following equation

$$b_n(\alpha)=\frac{1}{n}\mathrm{Tr}\left\{I\left[1+\gamma b_n(\alpha)\right]+(1-\gamma)+\frac{1}{1+\gamma b_n(\alpha)}AA^T\right\}^{-1},\gamma=\frac{m_n}{n}<1.$$

Under certain conditions the following assertion can be proven:

THEOREM 16.3. *If for every n, random components of the vector $\vec{\varepsilon}^T=\{\varepsilon_1,\dots,\varepsilon_n\}$ are independent, $\mathbf{E}\,\varepsilon_i=0,\ \mathbf{E}\,\varepsilon_i^2=n^{-1},\ i=1,\dots,n,\ 0<c_1\le m_n n^{-1}\le c_2<1$,*

$$\alpha_i\left(AA^T\right)\le c_3,\ i=1,\dots,m, D=I,$$

and the entries of the matrix X satisfy the conditions of Theorem 16.1, then

$$\lim_{n\to\infty}\left[G_{16}-\max_{\vec{c}^T\vec{c}\le 1}\mathbf{E}\left(\vec{c}-\vec{c}_\alpha\right)^T\left(\vec{c}-\vec{c}_\alpha\right)\right]=0.$$

16.4. G_{16} -estimator of regularized regression models errors. The resolvent method in the theory of experimental design, when the design matrix is a realization of a certain random matrix

Let us consider the regression model

$$\vec{y}=A\vec{c}+\vec{\varepsilon},\ \mathbf{E}\,\vec{\varepsilon}=\vec{0},\ \mathbf{E}\,\vec{\varepsilon}\vec{\varepsilon}^T=R_{m_n}.$$

In this case, in the expression

$$\max_{\vec{c}^T\vec{c}\leq 1}\mathbf{E}\left(\vec{c}-\vec{c}_\alpha\right)\left(\vec{c}-\vec{c}_\alpha\right)=\alpha\left\{\alpha+\lambda_{\min}\left[A^TA\right]\right\}^{-2} - \frac{\partial}{\partial\gamma}n^{-1}\mathrm{Tr}\left\{\alpha I+A^T\left(I+\gamma R\right)A\right\}^{-1}_{\gamma=0},\alpha>0. ,$$

a matrix A is unknown, but we know a realization of random matrix $X=A+\Xi$, and we want to estimate this expression for the unknown matrix A. Here the G_{16}-estimator is equal to

$$G_{16}=\alpha\left[\alpha+G_{28}^{\min}\right]^{-2}+\alpha\frac{\partial G_{27}\left(\alpha\right)}{\partial\alpha}+G_{27}\left(\alpha\right),$$

where the G_{27}-estimator of Stieltjes' transform (see Section 27)

$$\varphi\left(z,AA^T\right)=m^{-1}\mathrm{Tr}\left[AA^T-zI_{m_n}\right]^{-1}$$

is by definition the following expression:

$$G_{27}\left(z,XX^T\right)=\varphi\left(\hat{\theta}\left(z\right),XX^T\right)\left[1+\gamma\varphi\left(\hat{\theta}\left(z\right),XX^T\right)\right]^{-1},$$

$\hat{\theta}\left(z\right)$ is the measurable solution of the G_{27} equation

$$-\hat{\theta}\left(z\right)\left\{1+\frac{1}{n}\mathrm{Tr}\left[XX^T-\hat{\theta}\left(z\right)I_{m_n}\right]^{-1}\right\}^2 +\left(1-\frac{m_n}{n}\right)\left\{1+\frac{1}{n}\mathrm{Tr}\left[XX^T-\hat{\theta}\left(z\right)I_{m_n}\right]^{-1}\right\}=-z,$$

$G_{28}^{\min}$ is a consistent estimator for minimal eigenvalues $\alpha_m=\lambda_{\min}\left(AA^T\right)$ of the matrix AA^T which equals the minimal measurable solution x of the equation (see Section 28)

$$\lambda_{\min}\left(XX^T\right)=x\left\{1-\mathrm{Re}\left[\mathrm{i}\int_0^B\left\{\frac{\mathrm{e}^{|sp|}}{\pi}\int_{-A}^{A}\mathrm{Im}\,G_{27}\left(z\right)\mathrm{e}^{-\mathrm{i}tp}\mathrm{d}t\right\}\mathrm{e}^{-p(x-\mathrm{i}\varepsilon)}\mathrm{d}p\right]\right\}^2.$$

Under certain conditions the following assertion can be proven

Theorem 16.4. *If for every n, random components of vector $\vec{\varepsilon}^T=\{\varepsilon_1,\dots,\varepsilon_n\}$ are independent, $\mathbf{E}\,\varepsilon_i=0,\ \mathbf{E}\,\varepsilon_i^2=n^{-1},\ i=1,\dots,n,\ 0<c_1\leq m_nn^{-1}\leq c_2<1$,*

$$\alpha_i\left(AA^T\right)\leq c_3,\ i=1,\dots,m,$$

and the matrix X satisfies the conditions of Theorem 16.1, then

$$\lim_{n\to\infty}\left[G_{16}-\alpha\big\{\alpha+\lambda_{\min}[A^TA]\big\}^{-2}-\frac{\partial}{\partial\gamma}n^{-1}\mathrm{Tr}\big\{\alpha I+A^{\mathrm{T}}(I+\gamma R)A\big\}^{-1}_{\gamma=0}\right]=0.$$

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